

Large-Scale Epidemiological Simulation: Building New Capabilities on Renowned Science Foundations

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Over the last sixty years, Los Alamos National Laboratory (LANL), and particularly Theoretical Division, has developed foundational science and technologies—many internationally recognized. In times of changing national need, these foundational resources can be quickly mobilized to create new capabilities, providing LANL and the nation with new opportunities and needed resources. A prime

example is the transformation of the Scalable Parallel Short-range Molecular dynamics (SPaSM) simulation resource, combined with the foundational science of immune system modeling, into an unprecedented epidemiological simulation platform called EpiSPaSM.

To address the challenges of planning a response to intentional and/or natural outbreaks of pathogens contagious to humans or animals, the nation requires a single resource that 1) can utilize the highly resolved data being generated by syndromic and environmental monitoring systems, 2) examine many possible outcomes to capture the chaotic nature of an epidemic, and 3) capture the coupling between outbreaks on a regional level with outcomes at a national and world level.

Prior to EpiSPaSM, no epidemiological simulation could address all of these needs. The SPaSM code was ideally suited for this new application because of its proven capability to efficiently simulate molecular dynamics (i.e., processes at atomic resolution) of relatively large systems (billions of atoms). The ease in correspondence between

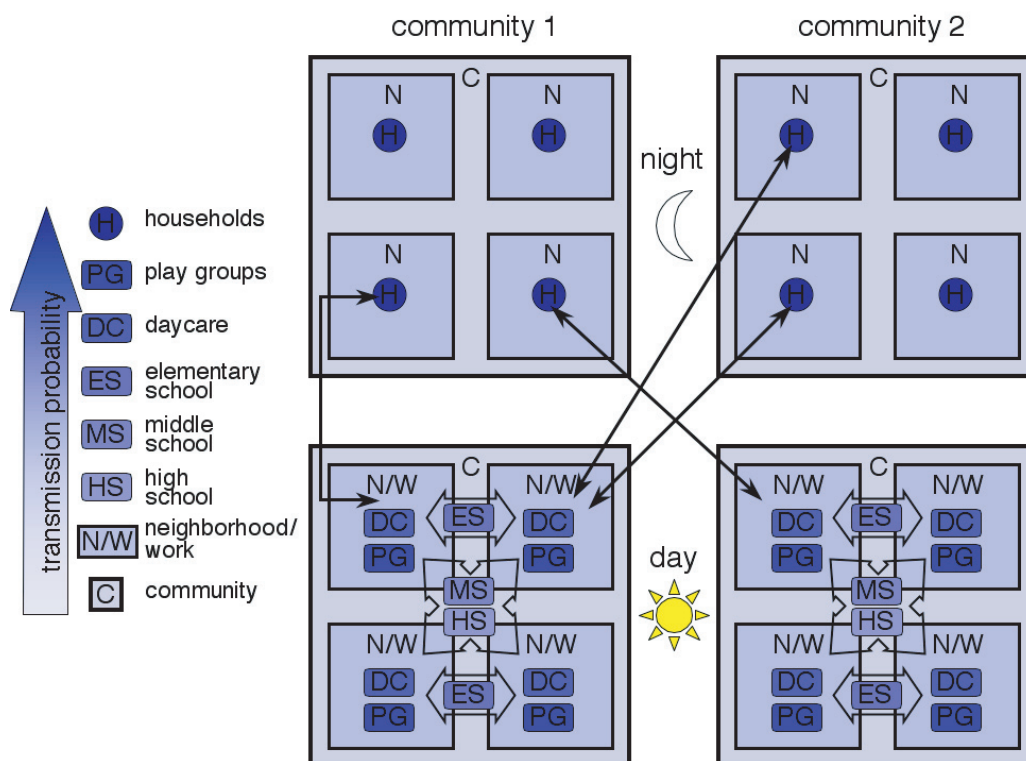


Figure 1—
 EpiSPaSM is based on a rich community model [1] of an epidemic with four neighborhoods, schools, homes, etc. (as listed in the left column). The communities are then connected together by individual movement between communities as guided by census data.

epidemiology and molecular dynamics was possible because the time evolution of both applications depend only upon localized (atom-atom or person-person) interactions. The computational immune system modeling at LANL provided the rich understanding of individual immune systems required by the high-resolution, individual-based model.

The core community model used in EpiSPaSM is a well-studied model that includes the essential features known to affect an epidemic (structured contact groups, age groups, individual immune responses, etc.), and is illustrated in Fig. 1. For a simulation of the entire U.S., this community model is replicated until a county's population is duplicated. Irregular travel is added based on detailed transportation statistics. Figure 2 shows the course of an epidemic with long-range travel for 1-out-of-10 people included in the simulation of 28 million people. (The 280 million people simulation is very similar.) EpiSPaSM has the capability to simulate a world epidemic (5 billion people), provided the necessary demographic and mobility data can be assembled.

In summary, the rapid development of EpiSPaSM, and its immediate contribution to national needs, would not have been possible without the long-standing investment by LANL in foundational technologies—the SPaSM large-scale simulation platform and computational immune system modeling.

[1] Halloran et al., *Science* **298**, 1428 (2002).

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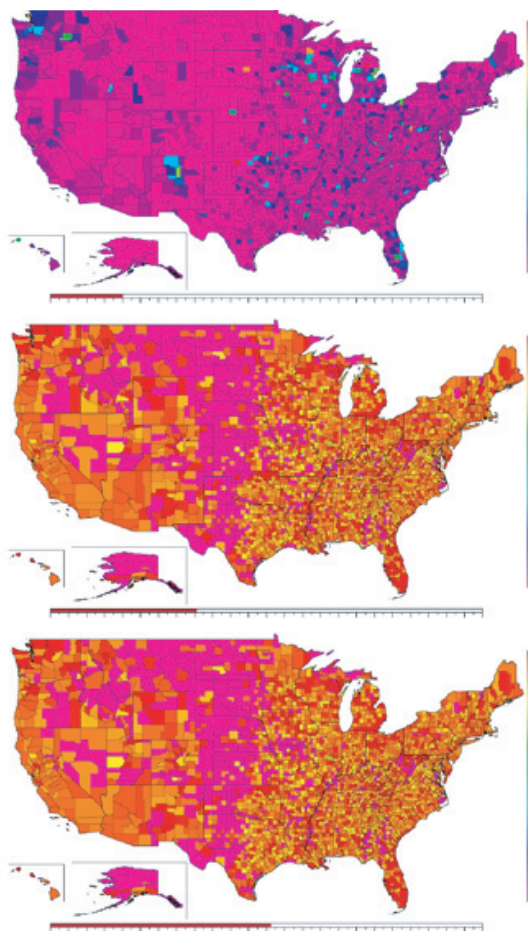


Figure 2—
Time evolution of the number of cumulative attack rate (the fraction of the population infected, purple: 0; red: 0.6). The smallpox epidemic is initiated by ten single adults in six locations in the U.S. The timebar shows approximately four years and one tick is four weeks.